

**Center for Mesoscale Transport Properties (m2m)**

**EFRC Director: Esther Takeuchi**

**Lead Institution: Stony Brook University**

**Start Date: August 2014**

***Mission Statement:*** *To understand and provide control of transport properties in complex battery systems with respect to multiple length scales, from molecular to mesoscale (m2m); to minimize heat and maximize work of electrical energy storage devices.*

At its essence, energy is the sum of heat and work:  $\Delta E = q + w$ . As such, the ultimate goal for any energy storage system is to maximize useful work ( $w$ ) and minimize the generation of waste heat ( $q$ ). During the operation of an energy storage system, ions and electrons are transported over multiple size domains where the sum of these processes leads to complex physics. Resistance evolves over time due to phase changes in the solids and changes in the composition and structure of the interfaces. These complicating factors must be considered to derive the full panoply of information needed for rational design and predictive modeling of materials useful in energy storage systems. While inefficiency can be approached at the macro level, emphasizing bulk parameters and bulk methods cannot fully interrogate or address the inherent heterogeneity of ion and electron flux contributing to the local resistance within an electrode and at the interfaces. In order to develop the capability to predict and ultimately control energy storage systems, these inefficiencies must be understood not just as a bulk property (heat), but rather as localized resistance at the molecular to mesoscale ( $m2m$ ) levels.

The goal of the  $m2m$  EFRC is to enable deliberate design of materials and components to achieve higher performing, longer life, and safer energy storage systems through acquisition of new fundamental knowledge about ion and electron transport and electron transfer properties of energy relevant materials, over multiple length scales, across interfaces and over time. The expected research outcomes are that the Center will provide the conceptual approaches to predict materials properties, processing outcomes, and functional characteristics which determine conduction and electron transfer properties, including the complexities of interfaces and time. The information gained will enable design of materials and systems to bridge the gap between theoretical energy content and functional energy delivery.

The Center will frame the key scientific investigations along three Scientific Inquiry Areas (SIA) that pose the following questions:

**1) What are the *fundamental limits* of ion and electron transport and electron transfer over multiple length scales?**

This question will be addressed by investigating transport and transfer phenomena for redox active moieties with several configurations. The roles of structure, crystallite size and particle size will be considered.

**2) How do the phenomena change across *multiple domains* including interfaces? Which systems level interactions are synergistic, independent, or antagonistic?**

The influence of physical properties, surface functionalization, and process on the transfer and transport properties and the function of composite electrodes will be explored.

**3) How do the transport phenomena evolve *over time* in systems not at equilibrium?**

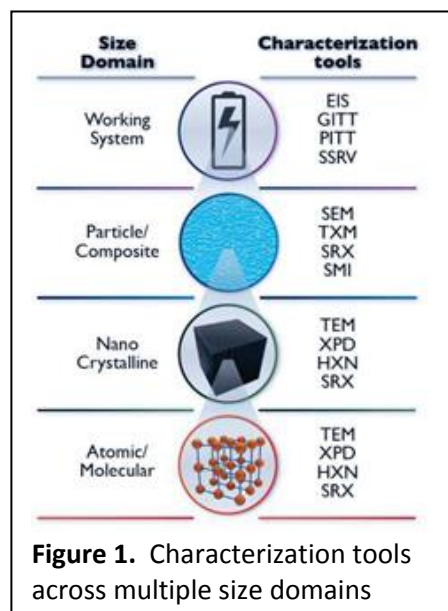
The effect of extended cycling on energy related solids will be studied to determine the effect of time.

The **m2m** Center will achieve the goals via:

- 1) integration of researchers in materials, characterization, theory and electrochemical systems interrogation.
- 2) use and development of microscopic and nanoscopic science based tools to provide characterization insights, highlighted in Figure 1.
- 3) synthetically tunable model redox active materials and electrolytes which will be shared among center members to facilitate interaction and data interpretation.
- 4) frequent communication and assessment.

The Center will access and utilize five notable facilities: the Advanced Energy Research and Technology Center (AERTC) and CEWIT at Stony Brook University, and the Interdisciplinary Science Building (ISB) including a 1200 sq ft dry room, National Synchrotron Light Source II (NSLS-II), and Center for Functional Nanomaterials (CFN) at Brookhaven National Laboratory.

AERTC will be the home base of the Center, providing access to a suite of new analytical instrumentation. CEWIT (Center of Excellence for Wireless Information Technology) will act as the data storage site for the Center.



Center for Mesoscale Transport Properties ( <i>m2m</i> )	
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